Optical Study of Non-Molecular and Insulator-Metal Transitions in Nitrogen Under Pressure

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Results: Optical spectroscopy techniques, including visible and near infrared (IR) Raman and synchrotron IR methods have been applied to study solid nitrogen at megabar pressures. We find that nitrogen becomes totally opaque above 150 GPa, accompanied by the disappearance of Raman and IR vibrational excitations, while new broad IR and Raman bands become visible. The transition shifts to higher pressures at low temperatures. Optical absorption measurements reveal that the semiconducting absorption edge responsible for the change of color is characterized by the presence of a wide Urbach-like tail and a high-energy (Tauc) region. These data are consistent with the dissociation of molecular nitrogen into a nonmolecular (possibly amorphous) phase. In the nonmolecular phase, the bandgap energy determined from Tauc plots decreases with pressure. Extrapolation of these measurements performed to 230 GPa indicates bandgap closure at about 280 GPa.

Conclusions: In conclusion, we present optical evidence for a transition of molecular nitrogen to a nonmolecular state. Vibrational and optical spectroscopic data indicate that the high-pressure phase is a narrowgap, disordered, and single-bonded phase.

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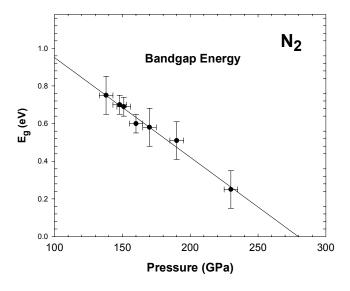


Figure 1. Band gap energy of solid nonmolecular semiconducting nitrogen as a function of pressure